Static and Dynamical Nonequilibrium Fluctuations

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Abstract: Various notions of fluctuations exist depending on the way one chooses to measure them. We discuss two extreme cases (continuous measurement versus long inter-measurement times) and we see their relation with entropy production and with escape rates. A simple explanation of why the relative entropy satisfies a Hamilton-Jacobi equation is added.

1. Introduction

All statistical mechanics originates from a fluctuation theory. For equilibrium statistical mechanics, there is the theory pioneered by Boltzmann, Planck and Einstein where probabilities are *derived* from macroscopic conditions. So then, if we know say the values of the energy, the particle number and perhaps a few other macroscopic quantities, we can *compute* specific heats, susceptibilities, etc. and see how they relate to fluctuations in energy, magnetization, etc. Moreover, thermodynamic potentials appear in the equilibrium fluctuation law to weigh the deviation from the macroscopic condition.
One would hope to achieve the same for nonequilibrium systems. Things are however more complicated here. To reach a nonequilibrium steady state, the system must be sufficiently open to an external world that permits the flow of energy or particles. As a consequence, there is no immediate analogue of the microcanonical ensemble from which all other equilibrium ensembles are derived. True, we could include that external world in our system to have again a closed total system but then we must deal with the problem of relaxation to equilibrium with special and long-lived nonequilibrium constraints.

In the present note, we deal with aspects of nonequilibrium fluctuations that, while clearly important, appear less known. One issue concerns the very notion of fluctuation. We emphasize an operational interpretation in which the nature of the fluctuation in fact depends on how we measure them. Secondly, we point out a couple of relations between fluctuation rates and thermodynamic or kinetic quantities. We explain the relation between relative entropy and entropy production

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and we suggest a new way of computing escape rates in nonequilibrium systems.

2. Fluctuations

Fluctuations can be large or small, steady or time-dependent; they obviously depend on the observable and they can e.g. measure deviations around the law of large numbers for a macroscopic quantity. Yet, in all events, it takes time to measure fluctuations. But if we speak about time-averages, we also need to specify how much time we leave after every observation. Especially so where time-correlations matter, we can expect to see relevant differences between more static (with large inter-times) and dynamic (with small inter-times) fluctuations.

Imagine we have a time-homogeneous steady state regime and ask what is the probability to see a particular value for some observable. E.g. for given nonequilibrium constraints, you ask how plausible it is to see a particular (local) density profile. That will be reflected in the frequency of occurence. You will probably want to make time-averages over a period T that is sufficiently long to see a steady value. Yet, for finite T there are always fluctuations. The point is now that these depend on the way of recording. To be more precise, think of a process $(X_t, t \geq 0)$, where X_t is the state of your system at time t (position, local density, magnetization, local kinetic energy,...). We fix $\tau > 0$; by a time-average we mean the average of $X_\tau, X_{2\tau}, X_{3\tau}, \ldots, X_T$. Over a long time T, we see the value x with a fraction

$$p_T^{(\tau)}(x) = \frac{1}{\lceil \frac{T}{\tau} \rceil} \sum_{k=1}^{\lceil \frac{T}{\tau} \rceil} \delta_{X_{k\tau}=x} \tag{2.1}$$

($\delta_{a=x} = 1$ when $a = x$ and is zero otherwise.) That is the relative frequency to observe x when measuring with time-intervals of length $\tau > 0$, for a duration T. There will appear two extremes: either $\tau \downarrow 0$ is very small, or $\tau \approx T$. The first type of fluctuations will be called *dynamical* and the second case corresponds to *static* fluctuations.

To be simple and to be specific, let us consider $(X_t)_{t\geq 0}$, a stationary ergodic Markov process, with invariant measure ρ. Have in mind steady state descriptions of mesoscopic systems via Langevin dynamics, or stochastic lattice gases etc. By the ergodicity, for $\boldsymbol{P}-$almost all states, $\lim_T p_T^{(\tau)} = \rho$, with $\boldsymbol{P}$ the law of the process. For finite T it could be that $p_T^{(\tau)}$ very much resembles a particular probability measure μ. Or, fixing an arbitrary probability law μ, we can ask how likely it is to observe it as the statistics of $(X_t)_t$. The theory of Donsker and

Varadhan [3, 2] gives an expression of the rate function

$$I_\tau(\mu) = -\inf_{g>0} \sum_{x,y} \mu(x) \log \frac{\sum_y g(y) P_\tau(y,x)}{g(x)} \tag{2.2}$$

where $P_\tau(x,y)$ are transition probabilities and the infimum is over all $g > 0$, appearing in the (logarithmic sense) limit $T \uparrow +\infty$ for (2.1):

$$\boldsymbol{P}[p_T^{(\tau)} \simeq \mu] \simeq e^{-T/\tau\, I_\tau(\mu)}, \qquad T \uparrow +\infty \tag{2.3}$$

Obviously, we can find the stationary distribution ρ from minimizing $I_\tau(\mu)$ over μ. That gives a variational characterization of ρ. Here is a special (limiting) case on which we will say more in Section 4. Taking the limit $\tau \downarrow 0$ corresponds to successive measurements with outcomes appearing with frequency

$$p_T^{(0)}(x) \equiv p_T(x) = \frac{1}{T} \int_0^T \delta_{X_t = x}\, \mathrm{d}t$$

i.e. a standard time-average. Then,

$$\boldsymbol{P}[p_T \simeq \mu] \simeq e^{-T I(\mu)} \tag{2.4}$$

where $I(\mu)$ is the Donsker-Varadhan functional that depends on the transition rates of the Markov process in the following sense:

$$I(\mu) = \lim_{\tau \downarrow 0} \frac{I_\tau(\mu)}{\tau} = \sum_{x,y} \mu(x)\, k(x,y) - \inf_{g>0} \sum_{x,y} \frac{g(y)\mu(x)}{g(x)} k(x,y) \tag{2.5}$$

In fact, this is a special case of a more general formula valid far beyond the restriction to finite state processes, namely,

$$I(\mu) = -\inf_{g>0} \boldsymbol{E}_\mu \Big[\frac{Lg}{g}\Big] \tag{2.6}$$

The expectation is over the process starting in the distribution μ and Lg is the generator of the process acting on a function g (over which we vary in (2.6)).

The variational principle originating from (2.5)-(2.6) appears rather 'unknown:' finding the stationary ρ amounts to finding the minimum of $I(\mu)$. Of course, even to evaluate $I(\mu)$ already another variation must be done, that over g. We discuss more of that problem in Section 4. The next section deals with the opposite limit $\tau \approx T$ of static fluctuations.

3. Varying the relative entropy

The limit $\tau \uparrow +\infty$ in the time-average (2.1) (with $T \uparrow +\infty$) corresponds to an infinite time separation between consecutive measurements. Then,

$$\lim_{\tau \uparrow +\infty} I_\tau(\mu) = S(\mu \,|\, \rho) \tag{3.1}$$

with $S(\mu \,|\, \rho)$ the relative entropy. For finite state spaces (and supposing that $\mu(x) = 0$ whenever $\rho(x) = 0$),

$$S(\mu \,|\, \rho) = \sum_x \mu(x) \log \frac{\mu(x)}{\rho(x)} \tag{3.2}$$

We recognize the expression as it figures as thermodynamic entropy or another related thermodynamic potential in Gibbsian descriptions of equilibrium systems.

The relative entropy (3.2) also appears often in treatments of nonequilibrium systems. We present two ways of looking at that.

3.1. **Relative entropy and entropy production.** It has often been emphasized that the relative entropy is a non-decreasing function for dissipative dynamics. Again, in our context of Markov processes on a finite state space,

$$\frac{\mathrm{d}}{\mathrm{d}t} S(\mu_t \,|\, \rho) \leq 0 \tag{3.3}$$

for the time-evolved probability distribution μ_t; $\rho_t = \rho$ as it is the invariant distribution. There is however need for more physical context if ever we want to interpret (3.3) as the positivity of the entropy production.
One possibility goes as follows.

The entropy production is the total change of the entropy in the world, system plus environment. Let us consider a transition $x \rightarrow y$ of the state of the system. We assume we have an entropy function S for the system, and the change of the entropy in the system is thus $S(y) - S(x)$. When the current between states x and y equals $j(x, y) = -j(y, x)$ (possibly depending on time), then the average instantaneous entropy production rate for the system is $\frac{1}{2}\sum_{x,y} j(x, y)\big[S(y) - S(x)\big]$. On the other hand, with some transitions $x \rightarrow y$ in the system, one imagines there corresponds a flow of particles or energy etc. to an external reservoir. These give rise to a change of entropy $S(x, y)$ in the environment. Hence, the total entropy production is $\frac{1}{2}\sum_{x,y} j(x, y)\,[S(x, y) + S(y) - S(x)]$. Let us see how to model that with the limited means of a Markov process with transition rates $k(x, y)$.

When the system is described at time t by the probability distribution μ_t, one can take as its entropy function $S(x) = -\log \mu_t(x)$. The expected rate of change of the system's entropy is thus

$$\dot{S}_s = \sum_{x,y} \mu_t(x) k(x, y) \big[-\log \mu_t(y) + \log \mu_t(x) \big] \tag{3.4}$$

Further, since we are modeling an open system dynamics, the ratio of transition rates $k(x, y)/k(y, x)$ should correspond to the entropy change

in the environment. E.g. if the states x and y carry different energies, $H(x) \neq H(y)$, then transitions $x \leftrightarrow y$ are only possible when the system exchanges energy with some heat bath. If the latter has inverse temperature $\beta(x,y)$, then $k(x,y)/k(y,x) = \exp[-\beta(x,y)\{H(y) - H(x)\}]$ and its logarithm gives the change of entropy in that reservoir. Therefore, under the distribution μ_t, the expected rate of change of entropy in the environment is

$$\begin{aligned}\dot{S}_e &= \sum_{x,y} \mu_t(x) k(x,y) \log \frac{k(x,y)}{k(y,x)} \\ &= \sum_{x,y} \mu_t(x) k(x,y) \log \frac{k(x,y)\mu_t(x)}{k(y,x)\mu_t(y)} - \dot{S}_s\end{aligned} \tag{3.5}$$

Upon adding (3.4) with (3.5), we obtain the total mean entropy production rate in the distribution μ_t

$$\dot{S} = \dot{S}_s + \dot{S}_e = \sum_{x,y} \mu_t(x) k(x,y) \log \frac{k(x,y)\mu_t(x)}{k(y,x)\mu_t(y)} \tag{3.6}$$

which is always non-negative.
Where do we see the relative entropy (3.2) in these expressions? When the stationary Markov dynamics satisfies the condition of (global) detailed balance, then

$$\frac{k(x,y)}{k(y,x)} = \frac{\rho(y)}{\rho(x)}$$

and following (3.6), the rate of total entropy production then equals

$$\begin{aligned}\dot{S} &= \sum_{x,y} \left[\mu_t(x)k(x,y) - \mu_t(y)k(y,x)\right] \log \frac{\mu_t(x)}{\rho(x)} \\ &= -\sum_{x,y} \frac{\mathrm{d}\mu_t(x)}{\mathrm{d}t} \log \frac{\mu_t(x)}{\rho(x)} \\ &= -\frac{\mathrm{d}}{\mathrm{d}t} S(\mu_t \,|\, \rho)\end{aligned} \tag{3.7}$$

where in the second equality we have used the Master-equation for the Markov process. Only when there is detailed balance, we can interpret (3.2) as (the negative of) the 'entropy of the world', the time derivative of which coincides with the (total) entropy production rate. One way of dealing with that last remark is to consider only closed systems that are already incorporating various reservoirs and in which the (total) dynamics is detailed balance with respect to some overall equilibrium distribution.

3.2. **Relative entropy and the Hamilton-Jacobi equation.** Let us assume that the Markov process has states in an interval of the form

$[A/\varepsilon, B/\varepsilon] \subset \mathbb{R}$ and rates

$$k(X,Y) = \frac{1}{\varepsilon}\, w(\varepsilon X, Y - X)$$

We have written capital letters to indicate that states X, Y represent values of a *macroscopic* observable(s), which is extensive in ε^{-1} proportional to the (great) number of particles. A standard example is (a continuous time version of) the Ehrenfest urn model. There a rescaled realization is $x \equiv \varepsilon X \in [0,1]$, possible transitions $r \equiv Y - X = \pm 1$, and the rescaled rates $w(x,1) = 1 - x$, $w(x,-1) = x$.

We consider the probability $p(x,t)$ to have a value $\varepsilon X = x$ at time t. It satisfies the Master-equation

$$\varepsilon \frac{\partial}{\partial t} p(x,t) = -\int \mathrm{d}r\; w(x,r)\, p(x,t) + \int \mathrm{d}r\; w(x - \varepsilon r, r)\, p(x - \varepsilon r, t) \tag{3.8}$$

We will be interested in the stationary distribution $p(x)$ verifying (3.8) with zero left-hand side. Let us assume that

$$p(x) \propto e^{-S(x)/\varepsilon} \tag{3.9}$$

for some function S, up to leading order as $\varepsilon \downarrow 0$. The entropy function S describes *static* stationary fluctuations similarly as the relative entropy (3.2) does. To see that, observe that when starting the process at time $-\tau$ from state a with $S(a) = 0$, then

$$\boldsymbol{P}[x(-\tau) = a, x(0) = b] \propto e^{-S(b)/\varepsilon}, \quad \tau \uparrow +\infty \tag{3.10}$$

similar to computing (2.3) for $T = \tau$.
There is an algorithm to directly compute S, obtained by rewriting (3.8) as

$$\varepsilon \frac{\partial}{\partial t} p(x,t) = -\int \mathrm{d}r\, \Big[1 - \exp\Big(-\varepsilon r \frac{\partial}{\partial x}\Big)\Big]\, w(x,r)\, p(x,t) \tag{3.11}$$

setting the left-hand side zero, and inserting formula (3.9) into (3.11) with $\varepsilon \downarrow 0$:

$$\int \mathrm{d}r\, w(x,r)\, \Big[1 - \exp\Big(r \frac{\partial}{\partial x} S(x)\Big)\Big] = 0 \tag{3.12}$$

We thus get a differential equation for the relative entropy!
As an example, again with $x \in [0,1]$, $r = \pm 1$, and $w(x,1) = 1 - x$, $w(x,-1) = x$, we see the solution $S(x) = x\, \log 2x + (1-x)\, \log 2(1-x)$, the relative entropy for a density x with respect to density $1/2$ in coin tossing.

The above scheme (with a somewhat different emphasis) was first mentioned in a paper of Kubo, Matsuo and Kitahara, [5]. We show how equation (3.12) can be seen as a (stationary) Hamilton-Jacobi

equation.
Formally, if we write

$$H(x,p) = \int \mathrm{d}r\, w(x,r)\, \big[1 - \exp(rp)\big] \tag{3.13}$$

then (3.12) takes the form

$$H\Big(x, \frac{\partial}{\partial x} S\Big) = 0 \tag{3.14}$$

We have to explain yet that the expression (3.13) is indeed the Hamiltonian corresponding to the path-space action. By that we mean that the probability to see the state x at time t when at time t_0 the state was x_0 is given by the path integral

$$\boldsymbol{P}(x,t\,|\,x_0,t_0) = \int_{x_0\to x} \mathrm{d}\omega\, \exp\Big[-\frac{1}{\varepsilon}\int_{t_0}^{t} \mathrm{d}s\, L(x(s),\dot{x}(s))\Big] \tag{3.15}$$

where we 'integrate' over all paths $\omega = (x(s);\, s \in [t_0,t])$ such that $x(t_0) = x_0$, $x(t) = x$, and the Lagrangian $L(x,\dot{x}) = p\,\dot{x} - H(x,p)$ is the Legendre transform of H. The reason for all that is the following.
In equation (3.10) we compute the left-hand side by the path integral (3.15) and assume that, as $\varepsilon \downarrow 0$, the integral over all paths ω can be approximated by the contribution of a single dominant path (which is the usual situation):

$$\begin{aligned}\boldsymbol{P}[x(-\tau) = a, x(0) = b] &= \int_{a\to b} \mathrm{d}\omega\, \exp\Big[-\frac{1}{\varepsilon}\int_{-\tau}^{0} \mathrm{d}s\, L(x(s),\dot{x}(s))\Big]\\ &\simeq \exp\Big[-\frac{1}{\varepsilon}\inf_{a\to b}\int_{-\tau}^{0} \mathrm{d}s\, L(x(s),\dot{x}(s))\Big]\end{aligned} \tag{3.16}$$

Hence,

$$S(b) = \inf_{a\to b}\int_{-\infty}^{0} \mathrm{d}s\, L(x(s),\dot{x}(s)) \tag{3.17}$$

which means that S is Hamilton's principal function for the Hamiltonian H associated to the Lagrangian L.

The idea of connecting the Hamilton-Jacobi equation with stationary fluctuations first appeared in [5], and was reinvented by [1] in the infinite-dimensional context. As we have shown above, these strategies amount to deriving a differential equation such as (3.12) for the relative entropy (such as S in (3.10)) from the (path-space) Lagrangian (such as L in (3.15)).

4. Escape rates

Recall the rate function (2.4)–(2.5) for the fluctuations corresponding to time-averages with continuous measurements. In general, this

is not so simple to compute explicitly, unless the Markov process is detailed balanced. Indeed, one checks that in that case of detailed balance with $k(x,y)\rho(x) = k(y,x)\rho(y)$, the minimizing g in (2.5) is given by $g(x) = \sqrt{\mu(x)/\rho(x)}$.

We now give an application of that same formula (2.4) but for a nonequilibrium situation: to compute the escape rate from a local equilibrium. To be specific, we consider a well-known nonequilibrium model with just one particle (or, what is the same, independent random walkers) hopping on a ring with N sites on which work is done. The jumps are nearest neighbor but they are biased in the sense that the rate for jumping clockwise is $k(x,x+1) = p$ while the rate for jumping counter clockwise is $k(x,x-1) = q$. It corresponds to an asymmetric random walk on a ring. The situation is sufficiently simple to understand that there is a unique stationary distribution ρ corresponding to the uniform placement of the walker on the ring: $\rho(x) = 1/N$. The question is again about fluctuations: what is the rate at which the particle will escape from a given subset of the ring?
It is most interesting to consider a connected subset $A = \{1,\ldots,n\}$ of $n < N$ sites. We are given a probability distribution μ localized on A, i.e., $\mu(x) \geq 0$ for $x \in A$ and $\sum_{x\in A}\mu(x) = 1$. Saying it differently, there is no mass outside A. Following the fluctuation formula (2.4) we want to find the rate $I(\mu)$ in the probability that the particle remains in A with occupation weights according to μ for the time T.

To solve for that escape rate $I(\mu)$ we must find the minimum in (2.5). However since μ is non-zero only on A, the only question is to minimize (over $g > 0$ on $\{1,\ldots,N\}$)

$$\sum_{x=1}^{n} \mu(x)\big[p\,\frac{g(x+1)}{g(x)} + q\,\frac{g(x-1)}{g(x)}\big]$$

Obviously the minimizer satisfies $g(x) = 0, x \notin A$ since all terms are non-negative anyway. So we are left with finding the minimal g for a functional $I'(\mu)$ corresponding to the dynamics on A for which again $k(x,x+1) = p, k(x,x-1) = q$ except when $x = 1$, respectively $x = n$, in which case the particle can only hop to the right, respectively the left. That new dynamics on A is however an equilibrium dynamics (when indeed $n < N$). One checks the condition of detailed balance for the distribution $\rho_A(x) \propto (p/q)^x, x \in A$. As a consequence we can take the minimizer g given as

$$g(x) = \sqrt{\mu(x)\left[\frac{q}{p}\right]^x}, \qquad x \in A$$

and the rate function for μ becomes, exactly, for $n < N$,

$$\begin{aligned} I(\mu) &= p + q - 2\sqrt{pq}\sum_{x=1}^{n-1}\sqrt{\mu(x)\mu(x+1)} \\ &= (\sqrt{p}-\sqrt{q})^2 + 2\sqrt{pq}\Big[1 - \sum_{x=1}^{n-1}\sqrt{\mu(x)\mu(x+1)}\Big] \end{aligned} \tag{4.1}$$

The minimum of that $I(\mu)$ is reached for the uniform distribution $\mu(x) = 1/n$ on A: we then have (4.1) $= (\sqrt{p}-\sqrt{q})^2 + 2\sqrt{pq}/n$. That is the inverse of the typical time that the particle feels the drive to escape from the set A. Fixing a time scale by putting $pq = 1$, we see that that escape time increases for $p = q$.

Another application of formula (2.4) concerns the relation with the so called minimum entropy production principle. Quite generally, the functional $I(\mu)$ is to first order in the driving and close to equilibrium an affine function of the entropy production rate. From that, we understand the minimum entropy production principle for Markov processes whose rates are a small perturbation from detailed balance rates, see [4, 7]. Details will follow in a separate publication, [8].

5. Final comments

The previous sections have given a short discussion of different types of nonequilibrium fluctuations. They vary from static to fully dynamical fluctuations. We have discussed a connection between the relative entropy as rate function for macroscopic fluctuations and a Hamilton-Jacobi equation. We have discussed a scheme to compute escape rates via the Donsker-Varadhan rate function for the dynamical fluctuations. Each time, we have seen relations with the entropy production. One final comment is in order however.

Recent years have seen a revival of attempts of constructing nonequilibrium statistical mechanics. It has however not been clear how far we have been moving beyond close to equilibrium considerations. In particular, the obsession with entropy production is probably related to the good experience we have with the situation around equilibrium. For descriptions further away from equilibrium, one will also need to deal with fluctuations of time-symmetric observables (which are not in the sector governed by the entropy production), see also the discussion in [6, 9]. In fact, we expect that the rate functions that have been considered in the present paper all carry information about time-symmetric currents when these rate functions are explored beyond first order around equilibrium.

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